

=> FILE REG

FILE 'REGISTRY' ENTERED AT 15:45:13 ON 17 JUL 2007

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=> D HIS

FILE 'LREGISTRY' ENTERED AT 15:36:59 ON 17 JUL 2007

L1 STR

FILE 'REGISTRY' ENTERED AT 15:40:32 ON 17 JUL 2007

L2 2 S L1

L3 19 S L1 FUL

SAV L3 BER482/A

FILE 'CAOLD' ENTERED AT 15:44:53 ON 17 JUL 2007

L4 2 S L3

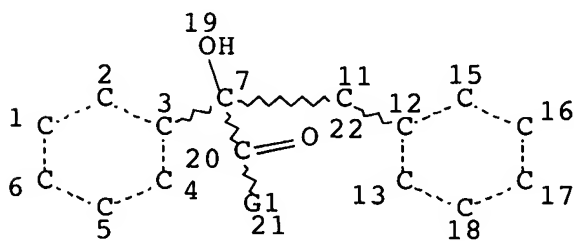
FILE 'ZCA' ENTERED AT 15:45:01 ON 17 JUL 2007

L5 16 S L3

FILE 'REGISTRY' ENTERED AT 15:45:13 ON 17 JUL 2007

=> D L3 QUE STAT

L1 STR



VAR G1=ME/ET/N-PR/I-PR/N-BU/I-BU/S-BU/T-BU

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L3 19 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 598 ITERATIONS

19 ANSWERS

SEARCH TIME: 00.00.01

=> FILE CAOLD

FILE 'CAOLD' ENTERED AT 15:45:23 ON 17 JUL 2007

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

=> D L4 1-2 ALL HITSTR

L4 ANSWER 1 OF 2 CAOLD COPYRIGHT 2007 ACS on STN

AN CA62:15760e CAOLD

TI studies on the electrolytic redn. of ketones - (III) electrolytic

redn. of aliphatic ketones-studies on cyclohexanone, (IV)

electrolytic redn. of unsatd. ketones-isophorone, (V) electrolytic

redn. of aryl alkyl diketones-studies on acetylbenzoyl, (VI)

electrolytic redn. of aromatic ketones-studies on fluorenone,

α -tetralone, acetophenone, and benzophenone

AU Arai, Toshio

IT 78-59-1 529-34-0 579-07-7 1636-34-6 1689-64-1

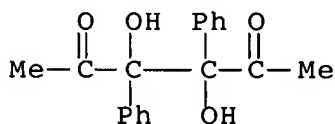
2888-11-1 3073-51-6 3073-53-8 3264-17-3

3427-06-3

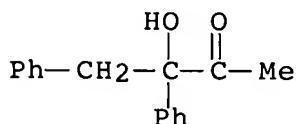
IT 3427-06-3

RN 3427-06-3 CAOLD

CN 2,5-Hexanedione, 3,4-dihydroxy-3,4-diphenyl- (7CI, 8CI, 9CI) (CA
INDEX NAME)



L4 ANSWER 2 OF 2 CAOLD COPYRIGHT 2007 ACS on STN
AN CA59:11299e CAOLD
TI analgesics-abs. configuration of α -(+)-4-dimethylamino-1,2-diphenyl-3-methyl-2-propionyxybutane, d-propoxyphene
AU Sullivan, Hugh R.; Beck, J. R.; Pohland, A.
IT 2214-31-5 3347-56-6 3536-29-6 5400-92-0 5725-99-5
5814-85-7 7001-80-1 23271-62-7 35030-49-0 54541-47-8
69262-53-9 83026-52-2 92553-77-0 92903-33-8
94756-79-3 97080-04-1
IT **69262-53-9**
RN 69262-53-9 CAOLD
CN 2-Butanone, 3-hydroxy-3,4-diphenyl- (7CI, 9CI) (CA INDEX NAME)



=> FILE ZCA
FILE 'ZCA' ENTERED AT 15:45:36 ON 17 JUL 2007
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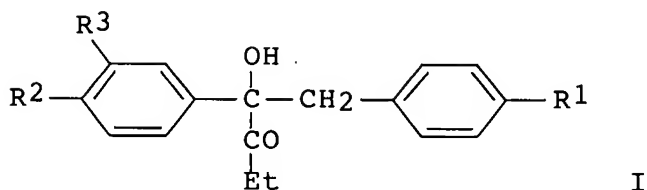
=> D L5 1-16 CBIB ABS HITSTR HITRN

L5 ANSWER 1 OF 16 ZCA COPYRIGHT 2007 ACS on STN
140:391638 Improvement in the storage stability of photoinitiators.
Ulrich, Thomas; Bolle, Thomas; Dietliker, Kurt; Wolf, Jean-Pierre;
Fuchs, Andre (Ciba Specialty Chemicals Holding Inc., Switz.). PCT
Int. Appl. WO 2004037799 A1 20040506, 49 pp. DESIGNATED STATES: W:
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO,
CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM,
HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL,
PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA,
UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH,
CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR,

NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2.

APPLICATION: WO 2003-EP50729 20031017. PRIORITY: CH 2002-1800
20021028.

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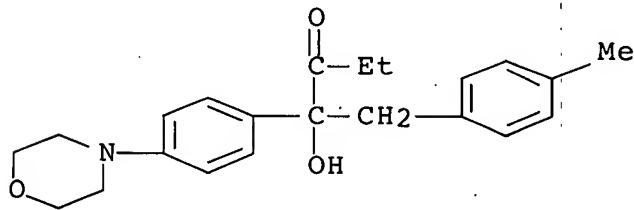
AB Compds. of formula (I), wherein R1 is hydrogen or alkyl; R2 is C1-C4 alkoxy or a morpholino radical; and R3 is hydrogen or C1-C4 alkoxy, are suitable for improving the soly. of specific photoinitiators in formulations and accordingly enhance the storage stability of formulations comprising a photoinitiator and compds. of formula I. Thus, I (R1 = Me, R2 = morpholino, R3 = H) was prepd. from trimethylsilyl cyanide, 4-morpholinobenzaldehyde, Et magnesium bromide, and 4-methylbenzyl bromide.

IT 685523-24-4P

(prepn. of storage stability improvers for photoinitiators)

RN 685523-24-4 ZCA

CN 3-Pentanone, 2-hydroxy-1-(4-methylphenyl)-2-[4-(4-morpholinyl)phenyl]- (9CI) (CA INDEX NAME)

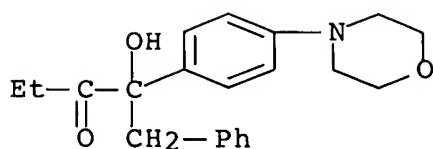


IT 685523-25-5 685523-26-6

(prepn. of storage stability improvers for photoinitiators)

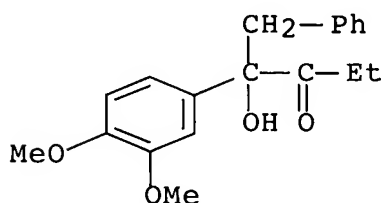
RN 685523-25-5 ZCA

CN 3-Pentanone, 2-hydroxy-2-[4-(4-morpholinyl)phenyl]-1-phenyl- (9CI)
(CA INDEX NAME)



RN 685523-26-6 ZCA

CN 3-Pentanone, 2-(3,4-dimethoxyphenyl)-2-hydroxy-1-phenyl- (9CI) (CA INDEX NAME)



IT 685523-24-4P

(prepn. of storage stability improvers for photoinitiators)

IT 685523-25-5 685523-26-6

(prepn. of storage stability improvers for photoinitiators)

L5 ANSWER 2 OF 16 ZCA COPYRIGHT 2007 ACS on STN

136:310039 Photochemical reduction of 1,2-diketones in the presence of

TiO₂. Park, Joon Woo; Hong, Mi Jeung; Park, Kwanghee Koh

(Department of Chemistry, Ewha Womans University, Seoul, 120-750, S.

Korea). Bulletin of the Korean Chemical Society, 22(11), 1213-1216

(English) 2001. CODEN: BKCSDE. ISSN: 0253-2964. OTHER SOURCES:

CASREACT 136:310039. Publisher: Korean Chemical Society.

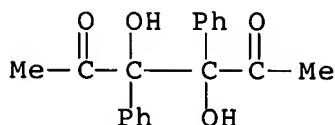
AB 1,2-Diketones, camphorquinone and 1-phenyl-1,2-propanedione, are converted to the corresponding α -hydroxy ketones in moderate to good yields by TiO₂-catalyzed photochem. reactions in deoxygenated alc. media. The redn. yield for 1-phenyl-1,2-propanedione is considerably increased by addn. of water or triethylamine.

IT 3427-06-3P

(photochem. redn. of camphorquinone and 1-phenyl-1,2-propanedione in the presence of TiO₂)

RN 3427-06-3 ZCA

CN 2,5-Hexanedione, 3,4-dihydroxy-3,4-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 3427-06-3P

(photochem. redn. of camphorquinone and 1-phenyl-1,2-propanedione in the presence of TiO₂)

L5 ANSWER 3 OF 16 ZCA COPYRIGHT 2007 ACS on STN

136:309820 Condensation of stereoisomeric 2-acetyl-2,3-diphenyloxiranes with ethyl trifluoroacetate. Tyvorskii, V. I.; Pukin, A. V.; Bobrov, D. N. (Belorussian State University, Minsk, Belarus). Chemistry of Heterocyclic Compounds (New York, NY, United States)(Translation of Khimiya Geterotsiklicheskikh Soedinenii), 37(5), 540-545 (English) 2001. CODEN: CHCCAL. ISSN: 0009-3122. OTHER SOURCES: CASREACT 136:309820. Publisher: Kluwer Academic/Consultants Bureau.

AB The reaction of rel-1-[(2R,3S)-1,2-Diphenyl-1-oxiranyl]ethanone with Et trifluoroacetate in the presence of sodium isopropoxide gave 3-hydroxy-2,3-diphenyl-6-trifluoromethyl-2,3-dihydro-4H-pyran-4-one. Under the same conditions rel-1-[(2R,3R)-1,2-Diphenyl-1-oxiranyl]ethanone forms 2-phenyl-5-(trifluoromethyl)-3-furanol as a result of retro-aldol cleavage of the initial cyclocondensation product.

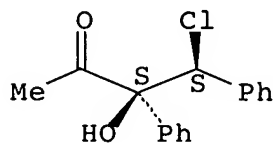
IT 411235-04-6P

(prepn. of 3-furanol derivs. by retro-aldol reaction of Et trifluoroacetate with rel-1-[(2R,3R)-1,2-diphenyl-1-oxiranyl]ethanone)

RN 411235-04-6 ZCA

CN 2-Butanone, 4-chloro-3-hydroxy-3,4-diphenyl-, (3R,4R)-rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



IT 411235-04-6P

(prepn. of 3-furanol derivs. by retro-aldol reaction of Et trifluoroacetate with rel-1-[(2R,3R)-1,2-diphenyl-1-

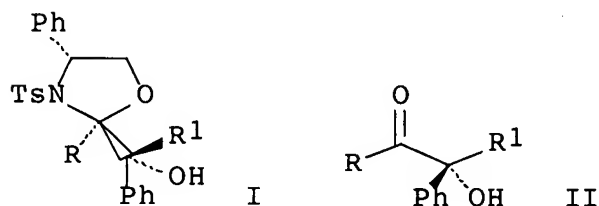
oxiranyl]ethanone)

L5 ANSWER 4 OF 16 ZCA COPYRIGHT 2007 ACS on STN

122:314143 Enantioselective synthesis of α -branched

α -hydroxy ketones via chiral N-sulfonyl-2-alkyl-2-cyano-1,3-oxazolidines. Harder, Timm; Loehl, Thorsten; Bolte, Michael; Wagner, Kerstin; Hoppe, Dieter (Organisch-Chemisches Inst., Univ. Muenster, Muenster, D-48149, Germany). Tetrahedron Letters, 35(40), 7365-8 (English) 1994. CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT 122:314143.

GI



AB The stereochem. homogeneous title oxazolidines, prepd. in two steps from orthoesters and N-tosylphenylglycinol, afford with two sequential Grignard addns. predominantly the tertiary alcs. I (R = Me, Et; R1 = Me, PhCH₂, allyl). Electrochem. detosylation, followed by aq. work up, yields enantiomerically enriched ketones II.

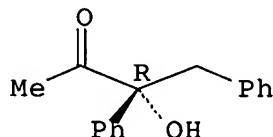
IT 161977-52-2P 161977-53-3P

(enantioselective synthesis of hydroxy ketones via chiral sulfonylalkylcyanooxazolidines)

RN 161977-52-2 ZCA

CN 2-Butanone, 3-hydroxy-3,4-diphenyl-, (R)- (9CI) (CA INDEX NAME)

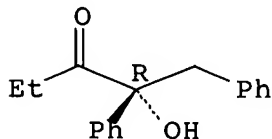
Absolute stereochemistry.



RN 161977-53-3 ZCA

CN 3-Pentanone, 2-hydroxy-1,2-diphenyl-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 161977-52-2P 161977-53-3P

(enantioselective synthesis of hydroxy ketones via chiral sulfonylalkylcyanooxazolidines)

L5 ANSWER 5 OF 16 ZCA COPYRIGHT 2007 ACS on STN

122:313938 The effects of counterion and solvent on the reactivity of nickel acylate complexes. La Duca, Melissa J. T.; Simunic, Joan L.; Hershberger, James W.; Pinhas, Allan R. (Department of Chemistry, University of Cincinnati, Cincinnati, OH, 45221-0172, USA).

Inorganica Chimica Acta, 222(1-2), 165-77 (English) 1994. CODEN: ICHAA3. ISSN: 0020-1693.

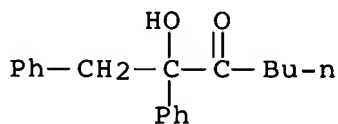
AB Nickel acylate complexes, which can be generated starting with a carbon, nitrogen or oxygen nucleophile, act as acyl anion equiv. and therefore are an excellent method of assembling complex org. mols. from readily available starting materials. In an effort to increase the synthetic utility of these easily formed reagents, a systematic study of the reactivity of the nickel acylate complex generated under a variety of conditions was performed. Those acylate complexes generated with a carbon based nucleophile, such as a Bu or Ph anion, show a large change in reactivity upon changing, for example, the solvent from THF to Et₂O or the counterion from Li⁺ to MgCl⁺. This reactivity change is due to a large change in the structure of the acylate complex with a different counterion or solvent, as detd. by IR and ¹³C NMR spectroscopy and by oxidn. potentials. In contrast, when a heteroatom nucleophile is used, such as a dialkyl amide or an alkoxide, the effect of a change in solvent or counterion on the structure, and therefore on the reactivity of the acylate complex, is minimal.

IT 163337-45-9P

(effects of counterion and solvent on the reactivity of nickel acylate complexes)

RN 163337-45-9 ZCA

CN 3-Heptanone, 2-hydroxy-1,2-diphenyl- (9CI) (CA INDEX NAME)



IT 163337-45-9P

(effects of counterion and solvent on the reactivity of nickel acylate complexes)

L5 ANSWER 6 OF 16 ZCA COPYRIGHT 2007 ACS on STN

114:5915 Regioreversed allylation in Lewis acid-mediated and photochemical addition reactions of unsymmetric α -diketones with allylic stannanes. Takuwa, Akio; Nishigaichi, Yutaka; Yamashita, Koichi; Iwamoto, Hidetoshi (Fac. Sci., Shimane Univ., Matsue, 690, Japan). Chemistry Letters (9), 1761-4 (English) 1990.

CODEN: CMLTAG. ISSN: 0366-7022. OTHER SOURCES: CASREACT 114:5915.

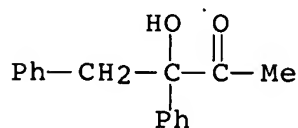
AB In the photochem. reaction of allyl- and benzyltrimethylstannane with unsym. α -diketones PhCOCOR, the allylic group was introduced to the benzoyl carbon in high or excellent selectivity, whereas the acyl carbon was allylated either exclusively or predominantly under BF₃-mediated reaction.

IT 69262-53-9P 130925-75-6P

(prepn. of)

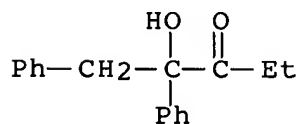
RN 69262-53-9 ZCA

CN 2-Butanone, 3-hydroxy-3,4-diphenyl- (7CI, 9CI) (CA INDEX NAME)



RN 130925-75-6 ZCA

CN 3-Pentanone, 2-hydroxy-1,2-diphenyl- (9CI) (CA INDEX NAME)



IT 69262-53-9P 130925-75-6P

(prepn. of)

L5 ANSWER 7 OF 16 ZCA COPYRIGHT 2007 ACS on STN

111:96764 Radical addition to carbonyl carbon promoted by aqueous titanium trichloride: stereoselective synthesis of α,β -dihydroxy ketones. Clerici, Angelo; Porta, Ombretta (Dip. Chim., Politec. Milano, Milan, 20133, Italy). Journal of

Organic Chemistry, 54(16), 3872-8 (English) 1989. CODEN: JOCEAH.

ISSN: 0022-3263. OTHER SOURCES: CASREACT 111:96764.

AB Ketyl radicals, formed by chemoselective Ti(III) redn. of α,β -dicarbonyl compds., add to the carbonyl carbon of aldehydes under mild conditions to afford α,β -dihydroxy ketones in good to excellent yields. Simple diastereoselectivity strongly depends on the bulk of groups bonded to both the ketyl radical and the aldehydic function. The relative configuration of two of the keto diols was established by single-crystal x-ray diffractometry.

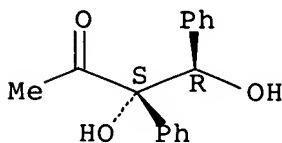
IT 122171-90-8P

(prepn. of)

RN 122171-90-8 ZCA

CN 2-Butanone, 3,4-dihydroxy-3,4-diphenyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 122171-90-8P

(prepn. of)

L5 ANSWER 8 OF 16 ZCA COPYRIGHT 2007 ACS on STN

102:131639 Facile preparation of 3-aryl-2-hydroxy-1-propanones by the Grignard-type addition of benzyl halides to 1,2-diketones mediated by metallic nickel. Inaba, Shinichi; Rieke, Reuben D. (Dep. Chem., Univ. Nebraska, Lincoln, NE, 68588-0304, USA). Synthesis (10), 844-5 (English) 1984. CODEN: SYNTBF. ISSN: 0039-7881. OTHER SOURCES: CASREACT 102:131639.

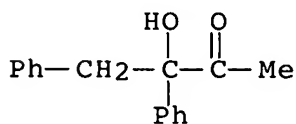
AB $RCH_2CR_1(OH)COR_2$ ($R = Ph, 4-MeC_6H_4, 3-F_3CC_6H_4, 4-FC_6H_4, 4-ClC_6H_4, 4-BrC_6H_4, 4-NCC_6H_4, 4-MeO_2CC_6H_4, 1-naphthyl$; $R_1, R_2 = Ph, Me$) were obtained in 35-83% yield by treating RCH_2R_3 ($R_3 = Cl, Br$) with R_1COCOR_2 in the presence of Ni.

IT 69262-53-9P

(prepn. of)

RN 69262-53-9 ZCA

CN 2-Butanone, 3-hydroxy-3,4-diphenyl- (7CI, 9CI) (CA INDEX NAME)



IT 69262-53-9P

(prepn. of)

L5 ANSWER 9 OF 16 ZCA COPYRIGHT 2007 ACS on STN

99:157554 Base catalyzed rearrangements involving ylide intermediates.

Part 18. Competing [1,2], [1,3], and [1,4] rearrangements of ammonium ylides. Chantrapromma, Kan; Ollis, W. David; Sutherland, Ian O. (Dep. Chem., Univ. Sheffield, Sheffield, S3 7HF, UK).

Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (5), 1049-61 (English) 1983.

CODEN: JCPRB4. ISSN: 0300-922X. OTHER SOURCES: CASREACT 99:157554.

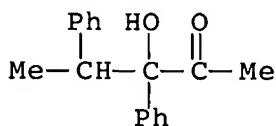
AB The mechanisms of the competing [1,2]-, [1,3]-, and [1,4]-rearrangements of benzyl- and phenylethylammonium ylides were studied. E.g., rearrangement of $\text{PhCOC-MeN+Me}_2\text{CH}_2\text{Ph}$ were largely intramol., with the intermolecularity of the [1,2]- and [1,3]-rearrangements being <28% and of the [1,4]-rearrangements being 14% in MeOH at 55°. Competing [1,2]- and [1,3]-rearrangements of optically active benzylammonium ylides, e.g. $\text{PhCOC-MeN+MeCHMePh}$, occurred with predominantly retention of configuration of the migrating group, but the intramol. stereoselectivity of the [1,2]-rearrangement was much greater than that of the [1,3]-rearrangement. The mechanism involves a radical pair path for all 3 rearrangements.

IT 69262-63-1P

(prepn. and degrdn. of)

RN 69262-63-1 ZCA

CN 2-Pentanone, 3-hydroxy-3,4-diphenyl- (9CI) (CA INDEX NAME)

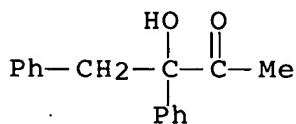


IT 69262-53-9P

(prepn. and redn. of)

RN 69262-53-9 ZCA

CN 2-Butanone, 3-hydroxy-3,4-diphenyl- (7CI, 9CI) (CA INDEX NAME)



IT 69262-60-8P 69303-25-9P 87258-78-4P

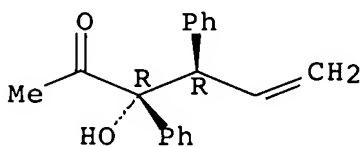
87258-79-5P

(prepn. of, by base-catalyzed rearrangement of acylammonium
ylide)

RN 69262-60-8 ZCA

CN 5-Hexen-2-one, 3-hydroxy-3,4-diphenyl-, (R*,R*)- (9CI) (CA INDEX
NAME)

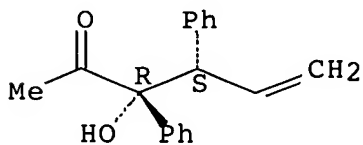
Relative stereochemistry.



RN 69303-25-9 ZCA

CN 5-Hexen-2-one, 3-hydroxy-3,4-diphenyl-, (R*,S*)- (9CI) (CA INDEX
NAME)

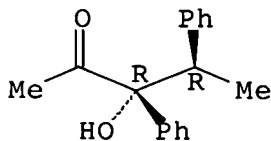
Relative stereochemistry.



RN 87258-78-4 ZCA

CN 2-Pentanone, 3-hydroxy-3,4-diphenyl-, (R*,R*)- (9CI) (CA INDEX
NAME)

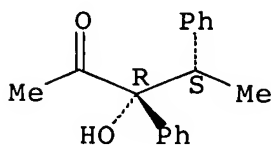
Relative stereochemistry.



RN 87258-79-5 ZCA

CN 2-Pentanone, 3-hydroxy-3,4-diphenyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 69262-63-1P

(prepn. and degrdn. of)

IT 69262-53-9P

(prepn. and redn. of)

IT 69262-60-8P 69303-25-9P 87258-78-4P

87258-79-5P

(prepn. of, by base-catalyzed rearrangement of acylammonium ylide)

L5 ANSWER 10 OF 16 ZCA COPYRIGHT 2007 ACS on STN

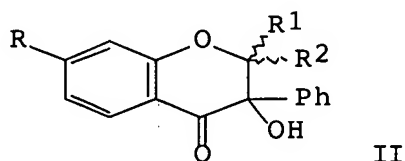
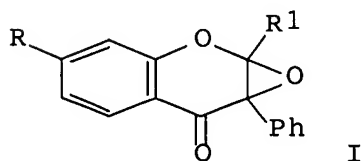
94:30492 Studies in the chemistry of chromone epoxides. Donnelly, John

A.; Keegan, John R.; Quigley, Killian (Chem. Dep., Univ. Coll.,

Dublin, Ire.). Tetrahedron, 36(11), 1671-80 (English) 1980. CODEN:

TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT 94:30492.

GI



AB Chromones and isoflavones were epoxidized by alk. H₂O₂ and their reactions studied. E.g., epoxide I (R = MeO, R₁ = H) underwent regioselective acid-catalyzed ring cleavage to 3-hydroxychromanone II (R = MeO, R₁ = α -OEt, R₂ = β -H), whereas acidic hydrolysis gave a 1,2-diol II (R = MeO, R₁ = OH, R₂ = H). A similar compd. was obtained by cyclizing 2-BzOC₆H₄COCHBr₂. In contrast, epoxide I (R = H, R₁ = Me) with BF₃·OEt₂ gave fluorohydrin II (R = H, R₁ = Me, R₂ = F) and acid- and base-

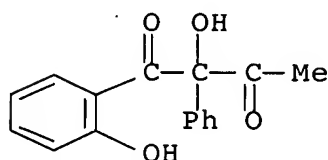
catalyzed hydrolysis gave a 1,3- and a 1,2-diketone, resp. This epoxide formed a cyclic sulfate with H₂SO₄.

IT 76182-84-8P

(prepn. of)

RN 76182-84-8 ZCA

CN 1,3-Butanedione, 2-hydroxy-1-(2-hydroxyphenyl)-2-phenyl- (9CI) (CA INDEX NAME)



IT 76182-84-8P

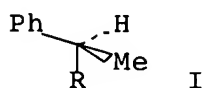
(prepn. of)

L5 ANSWER 11 OF 16 ZCA COPYRIGHT 2007 ACS on STN

90:86594 Stereoselectivities in competing [1,2] and [1,3]

rearrangements. Chantrapromma, Kan; Ollis, W. David; Sutherland, Ian O. (Dep. Chem., Univ. Sheffield, Sheffield, UK). Journal of the Chemical Society, Chemical Communications (15), 672-3 (English) 1978. CODEN: JCCCAT. ISSN: 0022-4936.

GI



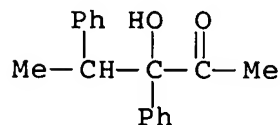
AB The competing intramol. [1,2] and [1,3] rearrangements of chiral ylide I (R = PhCOC-MeN+Me₂), generated by treatment of I (R = PhCOCHMeN+Me₂ BF₄⁻) with base, to give I [R = PhCOCMe(NMe₂), MeCOC(OH)Ph, resp.] are both stereoselective and occur with predominant retention of configuration of the migrating phenylethyl group. The stereoselectivity of the [1,2] rearrangement exceeds significantly that of the [1,3] rearrangement. The unusually high stereoselectivity of the [1,2] Stevens rearrangement is a consequence of the limited translational motion required within the radical pair before intramol. [1,2] coupling can occur.

IT 69262-63-1P

(prepn. and abs. configuration of)

RN 69262-63-1 ZCA

CN 2-Pentanone, 3-hydroxy-3,4-diphenyl- (9CI) (CA INDEX NAME)



IT 69262-63-1P

(prepn. and abs. configuration of)

L5 ANSWER 12 OF 16 ZCA COPYRIGHT 2007 ACS on STN

90:86448 Radical coupling products derived from ammonium ylides.

Competing [1,2], [1,3], and [1,4] anionic rearrangements.

Chantrapromma, Kan; Ollis, W. David; Sutherland, Ian O. (Dep. Chem.,

Univ. Sheffield, Sheffield, UK). Journal of the Chemical Society,

Chemical Communications (15), 670-1 (English) 1978. CODEN: JCCCAT.

ISSN: 0022-4936.

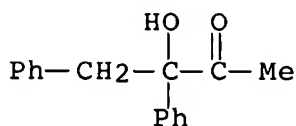
AB Thermal rearrangement of $\text{PhCOC-MeN+Me}_2\text{CH}_2\text{Ph}$ (I), generated by treating $\text{PhCOCHMeN+Me}_2\text{CH}_2\text{Ph Br-}$ with aq. NaOH, gave 86% $\text{PhCOCMe(CH}_2\text{Ph)NMe}_2$, 6% $\text{HOCMePhCOCH}_2\text{Ph}$ and 2% $\text{MeOCHPhCOCH}_2\text{Ph}$ by [1,2], [1,3] and [1,4] paths, resp. The intramolecularity of these processes was studied and showed that the rearrangement occurs via a radical-pair mechanism involving initial homolysis of I, followed by 3 possible modes of radical-pair recombination. For allylammonium ylides the no. of possible coupling modes is further increased.

IT 69262-53-9P 69262-60-8P 69303-25-9P

(prepn. of)

RN 69262-53-9 ZCA

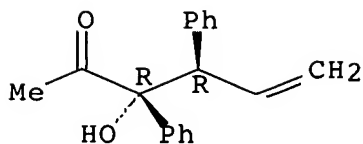
CN 2-Butanone, 3-hydroxy-3,4-diphenyl- (7CI, 9CI) (CA INDEX NAME)



RN 69262-60-8 ZCA

CN 5-Hexen-2-one, 3-hydroxy-3,4-diphenyl-, (R*,R*)- (9CI) (CA INDEX NAME)

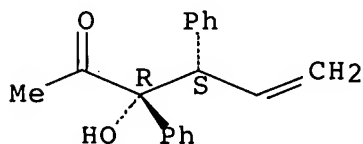
Relative stereochemistry.



RN 69303-25-9 ZCA

CN 5-Hexen-2-one, 3-hydroxy-3,4-diphenyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 69262-53-9P 69262-60-8P 69303-25-9P
(prepn. of)

L5 ANSWER 13 OF 16 ZCA COPYRIGHT 2007 ACS on STN

87:52424 Photochemistry of some cyclopropyl conjugated 1,2-diketones.

Part 2. Fragmentation reactions and reduction by aldehydes.

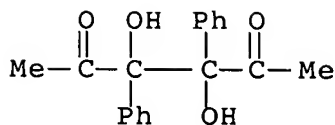
Kelder, J.; Cerfontain, H.; Van der Wielen, F. W. M. (Lab. Org. Chem., Univ. Amsterdam, Amsterdam, Neth.). Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (5), 710-14 (English) 1977. CODEN: JCPKBH. ISSN: 0300-9580.

AB The photochem. of 3 cyclopropyl conjugated and some related 1,2-diketones in C6H6 in the absence and presence of MeCHO or formylcyclopropane as H donor was studied. In C6H6 no photodecompn. occurred at $\lambda > 403$ nm, but at > 300 nm and < 403 nm the 1,2-diketones, with the exception of dicyclopropylethanedione (I), decompd. The products arise from initial bond rupture between the carbonyl groups, subsequent decarbonylation of part of the acyl radicals, and recombination. On irradiation of a I-biacetyl mixt., acyl interchange was obsd. The photoreaction of the 1,2-diketones in the presence of aliph. aldehyde gave dihydrodimers, α,α - diacylalkanols, and esters.

IT 3427-06-3P
(prepn. of)

RN 3427-06-3 ZCA

CN 2,5-Hexanedione, 3,4-dihydroxy-3,4-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 3427-06-3P
(prepn. of)

L5 ANSWER 14 OF 16 ZCA COPYRIGHT 2007 ACS on STN
82:42630 Photochemical reactions of some 1-aryl-1,2-propanediones.
Ogata, Yoshiro; Takagi, Katsuhiko (Fac. Eng., Nagoya Univ., Nagoya,
Japan). Bulletin of the Chemical Society of Japan, 49(7), 2255-9
(English) 1974. CODEN: BCSJA8. ISSN: 0009-2673.

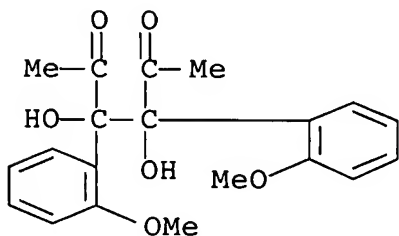
GI For diagram(s), see printed CA Issue.

AB Irradn. of 1-aryl-1,2-propanediones (I; R = H, p-OMe, o-OMe, O-Me) in 2-propanol gives pinacols or hydrols formed by redn. at the aroyl (but not acetyl) O. The products from I (R = o-Me) can also be accounted for by initial H abstraction from ortho Me by the aroyl carbonyl O. Their photoreactivities are discussed in relation to their electronic emission spectra and triplet configuration.

IT 53583-02-1P
(prepn. of)

RN 53583-02-1 ZCA

CN 2,5-Hexanedione, 3,4-dihydroxy-3,4-bis(2-methoxyphenyl)- (9CI) (CA
INDEX NAME)



IT 53583-02-1P
(prepn. of)

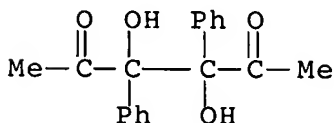
L5 ANSWER 15 OF 16 ZCA COPYRIGHT 2007 ACS on STN
62:88544 Original Reference No. 62:15760g-h Studies on the electrolytic
reduction of ketones. V. The electrolytic reduction of aryl alkyl
diketones. Studies on acetylbenzoyl. Arai, Toshio (Shinshu Univ.,
Nagano, Japan). Denki Kagaku, 30(3), 175-8 (Unavailable) 1962.
CODEN: DNKKA2. ISSN: 0366-9440.

AB MeCOCOPh (I) gave 2 half-wave potentials (-0.235 to -0.265, and -0.82 to -0.85 v.) at pH <3. At pH 3-8, the 1st wave shifted from -0.35 to -0.74 v., and the 2nd wave was not observed. No reductive half-wave was recognized at pH > 10. The remarkably low potential of the 1st wave at pH <3 was ascribed to the conjugation of C:O with the phenyl group. The 1st wave was concluded to be a 1-electron redn. wave on the basis of formation of α,β -diacetylhydrobenzoin (II), m. 118.5°. Use of Cu or Sn in redn. of 5 g. I in ethanolic 0.2N H₂SO₄ at 15-8° gave 1.5 or 2.2 g. II. No redn. product was obtained when Cd was used. Redn. of I with a Hg anode gave an organomercuric compd., m. 80° presumably PhCH₂CHMeHgCl.

IT 3427-06-3P, 2,5-Hexanedione, 3,4-dihydroxy-3,4-diphenyl-
(formation of, in acetylbenzoyl electrolytic redn.)

RN 3427-06-3 ZCA

CN 2,5-Hexanedione, 3,4-dihydroxy-3,4-diphenyl- (7CI, 8CI, 9CI) (CA
INDEX NAME)



IT 3427-06-3P, 2,5-Hexanedione, 3,4-dihydroxy-3,4-diphenyl-
(formation of, in acetylbenzoyl electrolytic redn.)

L5 ANSWER 16 OF 16 ZCA COPYRIGHT 2007 ACS on STN
59:61744 Original Reference No. 59:11299d-h,11300a-d Analgesics.

Absolute configuration of α -(+)-4-dimethyl-amino-1,2-diphenyl-3-methyl-2-propionoxybutane, d-propoxyphene. Sullivan, H. R.; Beck, J. R.; Pohland, A. (Eli Lilly & Co., Indianapolis, IN). Journal of Organic Chemistry, 28(9), 2381-5 (Unavailable) 1963. CODEN: JOCEAH. ISSN: 0022-3263.

GI For diagram(s), see printed CA Issue.

AB α -(+)-Me₂NCH₂CHMeCPh(CH₂Ph)O₂CEt.HCl (I) (15 g.) and 135 mL. 5N HCl was refluxed 2 h. and concd. to dryness to give 8.5 g. (--)Me₂NCH₂CHMeCPh:CHPh.HCl (II), m. 189-90° (MeOH-EtOAc), [α] (all 25/D) -33.7° (c 1, H₂O). Similarly, 50 g. α -(--) isomer of I gave 21 g. II (--) isomer (III), m. 189-90°, [α] 34.3° (c 1, H₂O). Into 25 g. II, 150 mL. MeOH, and 1100 mL. EtOAc at -20° was passed O₃ in excess; the whole added to 250 mL. ice-H₂O, kept overnight, the MeOH and EtOAc distd. in vacuo, the aq. soln. washed with Et₂O (concn. of these gave BzH), the aq. soln. treated with excess aq. NH₃, extd. with Et₂O, and the Et₂O, exts. dried and treated with dry HCl gave 8 g. (--)Me₂NCH₂CHMeBz.HCl (IV), m. 153-4° (MeOH-EtOAc), [α] -47° (c 1, H₂O). To 11.8 g. IV, 130 g. anhyd. Na₂HPO₄, and 300 mL. CH₂Cl₂ at 0-5° was added CF₃-CO₃H [from 50.8 g. (CF₃CO)₂O, 8.2 mL. 90% H₂O₂, and 100 mL. CH₂Cl₂, at 0°]; the whole stirred 1 h. (temp. rise to 10°), the solid mixt. kept 4 h. at room temp., 200 mL. H₂O added, the CH₂Cl₂ phase sepd., evapd. to dryness, the residue dissolved in 100 mL. 2N HCl, washed, treated with excess concd. aq. NH₃ and extd. with Et₂O and the dried Et₂O soln. treated with dry HCl gave 3.8 g. (--)Me₂NCH₂CHMeOBz.HCl, m. 160-1° (MeOH-

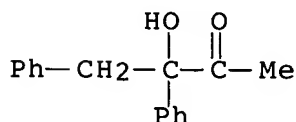
EtOAc), $[\alpha] -62.8^\circ$ (c 1, H₂O). D(-)-H₂NCH₂CH-(OH)Me.HCl (2.7 g.), 1.6 g. HCO₂Na, 8.3 g. 100% HCO₂H, and 6.7 g. 37% HCHO were refluxed 14 h. to give 3.13 g. hygroscopic D(--)-Me₂NCH₂CH(OH)Me.HCl (V), $[\alpha] -44.5^\circ$ (c 1, MeOH); V, 7.1 g. BzCl, 25 mL. Et₃N, and 80 mL. CHCl₃ refluxed 1 h. gave 4.2 g. Me₂NCH₂CH(OBz)Me, HCl, m. 160-1° (MeOH-EtOAc), $[\alpha] -63.3^\circ$ (c 1, H₂O). I (370 g.), 4.5 l. MeOH, and 650 mL. 30% H₂O₂ kept 48 h. at room temp., the whole evapd. to dryness, 0.4 g. PtO₂ added (caution), filtered, the filtrate evapd. to dryness, and the residue in 2 l. EtOAc treated with 40 g. HCl in 1 l. EtOAc gave 370 g. I N-oxide-HCl (VI), m. 186-7° (MeOH-EtOAc), $[\alpha] 20.2^\circ$ (c 2, MeOH); VI in 1500 mL. H₂O satd. with K₂CO₃ and extd. with Et₂O gave 320 g. N-oxide (VII); VII heated slowly at 0.5 mm. to 140°, kept 0.5 h. at 140°, the whole cooled, dissolved in Et₂O and the Et₂O soln. washed, dried, concd. and distd. gave 200 g. (+)-CH₂:CMeCPh(CHPh)O₂CEt (VIII), b_{0.6} 152°, n_{25D} 1.5466, $[\alpha] 97^\circ$ (c 1.3, Me₂CO) (the cold trap from the pyrolysis contained Me₂NHOH). VIII (45 g.) in 1 l. EtOAc at -50° and O₃ to blue color, the whole poured into ice-H₂O, kept overnight, dil. aq. NaHSO₃ added, dropwise, to neg. starch-iodide test, the EtOAc soln. sepd., washed and dried gave 41 g. (+)-AcCPh-(O₂CEt)CH₂Ph (IX), b_{0.5} 156-7°, $[\alpha] 182.7^\circ$ (c 1.1, Me₂CO). IX (32.5 g.), 1 l. 5N HCl, and 1 l. EtOH refluxed 20 h. gave 21.9 g. (+)-AcC(OH)PhCH₂Ph (X), b_{0.5} 148°, n_{25D} 1.5660, $[\alpha] 141^\circ$ (c 1.3, EtOH). To 60 g. X in 200 mL. glacial AcOH was added, dropwise, 45 g. Br in 100 mL. glacial AcOH, and the whole stirred 1 h. and evapd. to dryness in vacuo; the residue in 600 mL. C₅H₅N heated 1 h. at 100°, the whole concd., and the residue and 60 g. NaOH in 900 mL. H₂O heated 2 h. at 100° gave 20 g. (-)-PhCH₂C(OH)PhCO₂H (XI), m. 145-6° (aq. EtOH), $[\alpha] 13.7^\circ$ (c 3.5, EtOH). XI (18 g.), 40 g. Ag₂O and 200 mL. MeI refluxed and stirred 3 h. gave 15 g. Me ester (XII), m. 102-3° (Et₂O-petr. ether), $[\alpha] -32.4^\circ$ (c 3.4, CHCl₃). Abs. EtOH, (200 mL.) and 60 g. freshly prepd. W-2 Raney Ni, shaken first with 40 lb./in.² H, 8 g. XII added, and the whole refluxed 8 h., filtered, the residue from the concn. of the filtrate dissolved in 40 mL. petr. ether, 1.4 g. XII which sepd., filtered off, the filtrate evapd. and the residue distd. gave 6 g. (+)-PhCH₂CHPhCO₂Me (XIII), b_{0.2} 123-4°, n_{25D} 1.5518, $[\alpha] -90.5^\circ$ (c 4.6, CHCl₃). To 1.7 g. LiAlH₄ in 110 mL. anhyd. Et₂O was added 10.2 g. XIII in 40 mL. Et₂O, dropwise, and the whole refluxed 3 h. to give 7.8 g. (+)-PhCH₂CHPhCH₂OH, b_{0.2} 128°, n_{25D} 1.5742, $[\alpha] 76.3^\circ$; tosylate (XIV) (prepd. in C₅H₅N), m. 89-90° (Me₂CO-petr. ether), $[\alpha] 40.2^\circ$ (c 2.4, Me₂CO). XIV (7.4 g.), 16.5 g. NaI, and 200 mL. anhyd. Me₂CO refluxed and stirred 20 h. gave 6.35 g. (+)-PhCH₂CHPhCH₂I (XV), m. 54-5° (petr. ether), $[\alpha] 16.6^\circ$ (c 3.9, EtOH); XV, 3.0 g. NaHCO₃, 150 mL. abs. EtOH, and 5 g. Pd-C hydrogenated 10 h. at 25° gave 2.6 g. (+)-PhCH₂CHPhMe, b_{0.3} 85°, n_{25D} 1.5558, $[\alpha] 76.7^\circ$ (c 2.3, CHCl₃). (-)-threo-PhCH(OH)CHPhMe (1.4 g.) added to 100 mL. abs. EtOH and 30 g. W-2 Raney Ni, shaken first in H as above, and the whole refluxed 8 h. gave 1.15 g. D(-)-PhCH₂CHPhMe, b_{0.5} 88°, n_{25D} 1.5553, $[\alpha] -76.3^\circ$ (c 2.2, CHCl₃). The abs. configuration of I is (2S,3R).

IT 69262-53-9P, 2-Butanone, 3-hydroxy-3,4-diphenyl-

(prepn. of)

RN 69262-53-9 ZCA

CN 2-Butanone, 3-hydroxy-3,4-diphenyl- (7CI, 9CI) (CA INDEX NAME)



IT 69262-53-9P, 2-Butanone, 3-hydroxy-3,4-diphenyl-
(prepn. of)